AUTHOR INDEX TO VOLUME 122

Abramczyk, H. and J. Michalak, Conformational analysis of 2-chloro-5,5-dimethyl-2-oxo-1,3,2-dioxaphosphorinane by molecular dynamics method. Vibrational dephasing and interaction-induced IR absorption 122 (1988) 317
Anastasi, C., see S. Rettrup 122 (1988) 45
Andrews, D.L. and N.P. Blake, Laser-induced molecular orientation effects in vibrational resonance-Raman spectroscopy 122 (1988) 169

Baerends, E.J., see P.M. Boerrigter 122 (1988) 357
Barth, A., see J. Schirmer 122 (1988) 9
Bednarek, G., see J. Wildt 122 (1988) 463
Berry, M.T., C. Schwieters and F.S. Richardson, Optical absorption spectra, crystal field analysis, and electric dipole intensity parameters for europium in $Na_3[Eu(ODA)_3]\cdot 2NaClO_4\cdot 6H_2O$ 122 (1988) 105
Berry, M.T., C. Schwieters and F.S. Richardson, Circular dichroism spectra and electronic rotatory strengths of the europium 4f→4f transitions in $Na_3[Eu(ODA)_3]\cdot 2NaClO_4\cdot 6H_2O$ 122 (1988) 125
Blake, N.P., see D.L. Andrews 122 (1988) 169
Boerrigter, P.M., E.J. Baerends and J.G. Snijders, A relativistic LCAO Hartree- Fock–Slater investigation of the electronic structure of the actinocenes $M(COT)_2$, M=Th, Pa, U, Np and Pu 122 (1988) 357
Botschwina, P., see J. Senekowitsch 122 (1988) 375
Botschwina, P., see U. Mänz 122 (1988) 387
Bowers, M.S., see Q.F. Pan 122 (1988) 193
Brion, C.E., see C.L. French 122 (1988) 247
Bull, T.E., Fokker–Planck–Langevin and extended diffusion models of internal rotation in molecules. I. Symmetric internal rotor. Chem. Phys. 121 (1988) 1. Erratum 122 (1988) 168

Cammi, R., F.J. Olivares del Valle and J. Tomasi, Decomposition of the interaction energy with counterpoise corrections to the basis set superposition error for dimers in solution. Method and application to the hydrogen fluoride dimer 122 (1988) 63
Carter, S., see J. Senekowitsch 122 (1988) 375
Chrapeć, J., S.J. Rzoska and J. Zioło, Properties of the nonlinear dielectric effect in critical nitrobenzene in *n*-alkane solutions in a broad range of temperatures 122 (1988) 471
Chupka, W.A., see P.J. Miller 122 (1988) 395
Colpa, J.P., Contribution to the theory of time-resolved microwave-induced optical nuclear polarization. Theoretical extremum values for the induced polarization 122 (1988) 29
Corvaja, C., see A.L. Maniero 122 (1988) 327

Davidson, E.R., see C.L. French 122 (1988) 247
De Haas, M.P., see P.C.M. Weisenborn 122 (1988) 147
Diercksen, G.H.F., see A.J. Sadlej 122 (1988) 297

Drexhage, K.H., see N.P. Ernsting 122 (1988) 431
Duran, M., Y. Yamaguchi, R.B. Remington and H.F. Schaefer III, Analytic energy second derivatives for paired-excited multi-configuration self-consistent-field wavefunctions. Application of the PEM CSCF model to H_2O, CH_2, HCN, HCCH, H_2CO, NH_3, CH_4, and C_2H_4 122 (1988) 201

Eland, J.H.D., see P.J. Miller 122 (1988) 395
Ernsting, N.P., M. Kaschke, J. Kleinschmidt, K.H. Drexhage and V. Huth, Sub-picosecond time-resolved intramolecular electronic energy transfer in bichromophoric rhodamine dyes in solution 122 (1988) 431

Fain, B., V. Fleurov and S.H. Lin, Intermolecular energy transfer in infrared-laser-induced desorption 122 (1988) 17
Fink, E.H., see J. Wildt 122 (1988) 463
Fleurov, V., see B. Fain 122 (1988) 17
French, C.L., C.E. Brion and E.R. Davidson, A study of the valence orbitals of H_2S by electron momentum spectroscopy: quantitative comparisons using Hartree–Fock limit and correlated wavefunctions 122 (1988) 247

Gisby, J.A. and S.H. Walmsley, A theoretical investigation of the variation with pressure of the ultraviolet absorption spectrum of crystalline anthracene 122 (1988) 271

Herman, A., An improved Sandorfy C method for permethylpolysilanes 122 (1988) 53
Huth, V., see N.P. Ernsting 122 (1988) 431

Kaschke, M., see N.P. Ernsting 122 (1988) 431
Kemister, G. and N.H. March, Relation between total energy and orbital energy sum in molecules: atomic and bonding contributions 122 (1988) 39
Kharlamov, B.M., see N.I. Ulitsky 122 (1988) 1
Kleinschmidt, J., see N.P. Ernsting 122 (1988) 431
Klochikhin, V.L. and S.Ya. Pshezhetskii, Diffusion-controlled kinetics of systems containing a finite number of reacting particles 122 (1988) 279
Kudo, T. and S. Nagase, Jahn–Teller distortions of SiH_4^+ and $Si(CH_3)_4^+$. 122 (1988) 233
Kuritsyn, Yu.A., G.N. Makarov, I. Pak and M.V. Sotnikov, Tunable diode laser studies of collisionless infrared excitation of SF_6 and NH_3 molecules 122 (1988) 97
Kushawaha, V., A. Michael and M. Mahmood, Observation of excited state species due to N^+/N_2^+ and CH_3HgX (X=Cl, Br, I) collisions 122 (1988) 183

Latajka, Z. and S. Scheiner, Structure, energetics, and vibrational spectra of H-bonded systems. Dimers and trimers of HF and HCl 122 (1988) 413
Leroy, J.P., see R. Wallace 122 (1988) 75
Levy, B., see J. Ridard 122 (1988) 403
Liedenbaum, C., S. Stolte and J. Reuss, Multi-photon excitation of a beam of SF_6 molecules pumped and probed by cw CO_2 lasers 122 (1988) 443
Lin, S.H., see B. Fain 122 (1988) 17

Mahmood, M., see V. Kushawaha 122 (1988) 183

Makarov, G.N., see Yu.A. Kuritsyn 122 (1988) 97
Maniero, A.L., C. Corvaja and L. Pasimeni, Proton ENDOR spectra of phenanthrene–TCNB triplet traps in single crystals of naphthalene–TCNB 122 (1988) 327
Mänz, U., P. Rosmus, H.-J. Werner and P. Botschwina, The first excited triplet state of NH_3 122 (1988) 387
March, N.H., see G. Kemister 122 (1988) 39
Michael, A., see V. Kushawaha 122 (1988) 183
Michalak, J., see H. Abramczyk 122 (1988) 317
Miller, P.J., W.A. Chupka and J.H.D. Eland, Vibrationally autoionizing Rydberg states of NH_3 122 (1988) 395
Millié, P., see J. Ridard 122 (1988) 403

Nagase, S., see T. Kudo 122 (1988) 233
Nguyen, M.T., N.V. Riggs and L. Radom, Molecular structure and spectroscopic properties of carbodiimide (HN–C–NH) 122 (1988) 305
Nyeland, C. and J.P. Toennies, Modelling of repulsive potentials from charge density distributions: a new site–site model applied to inert gas atoms with the diatomic molecules H_2, N_2, O_2 122 (1988) 337

Oddershede, J. and J.R. Sabin, Calculation of rotational *g*-factors and magnetic susceptibilities of H_3^+ 122 (1988) 291
Oddershede, J., see A.J. Sadlej 122 (1988) 297
Olivares del Valle, F.J., see R. Cammi 122 (1988) 63

Pagsberg, P., see S. Rettrup 122 (1988) 45
Paidarová, I. and J. Vojtík, Non-adiabatic interaction in the autoionizing singlet $He^*–H_2$ system 122 (1988) 89
Pak, I., see Yu.A. Kuritsyn 122 (1988) 97
Pan, Q.F., M.S. Bowers and K.T. Tang, The interaction potential and diffusion coefficients of sodium in neon 122 (1988) 193
Papadimitriou, D., H.V. Schwarz and B. Schramm, Vibrational relaxation of HBr($v=1$) in D_2 between 300 and 140 K 122 (1988) 141
Pasimeni, L., see A.L. Maniero 122 (1988) 327
Personov, R.I., see N.I. Ulitsky 122 (1988) 1
Pshezhetskii, S.Ya., see V.L. Klochikhin 122 (1988) 279

Radom, L., see M.T. Nguyen 122 (1988) 305
Remington, R.B., see M. Duran 122 (1988) 201
Rettrup, S., P. Pagsberg and C. Anastasi, Ab initio configuration interaction study of the Rydberg states of the hydroxymethyl radical CH_2OH 122 (1988) 45
Reuss, J., see C. Liedenbaum 122 (1988) 443
Richardson, F.S., see M.T. Berry 122 (1988) 105
Richardson, F.S., see M.T. Berry 122 (1988) 125
Richert, R., Dynamics of a polymer matrix probed by the ring closure of merocyanine 122 (1988) 455
Ridard, J., B. Levy and P. Millié, Theoretical investigation of the dissociation of OCS^{2+} in the process $OCS(X^1\Sigma^+)+h\nu \rightarrow OCS^{2+} \rightarrow CO^+(X^2\Sigma^+)+S^+(^4S)$ 122 (1988) 403
Riggs, N.V., see M.T. Nguyen 122 (1988) 305

Rosmus, P., see J. Senekowitsch 122 (1988) 375
Rosmus, P., see U. Mänz 122 (1988) 387
Rzoska, S.J., see J. Chrapeć 122 (1988) 471

Sabin, J.R., see J. Oddershede 122 (1988) 291
Sabin, J.R., see A.J. Sadlej 122 (1988) 297
Sadlej, A.J., G.H.F. Diercksen, J. Oddershede and J.R. Sabin, How reliable is the theoretical structure of SiC_2? 122 (1988) 297
Schaefer III, H.F., see M. Duran 122 (1988) 201
Scheiner, S., see Z. Latajka 122 (1988) 413
Schirmer, J., A. Barth and F. Tarantelli, Theoretical study of K-shell excitations in formaldehyde 122 (1988) 9
Schramm, B., see D. Papadimitriou 122 (1988) 141
Schwarz, H.V., see D. Papadimitriou 122 (1988) 141
Schwieters, C., see M.T. Berry 122 (1988) 105
Schwieters, C., see M.T. Berry 122 (1988) 125
Senekowitsch, J., A. Zilch, S. Carter, H.-J. Werner, P. Rosmus and P. Botschwina, Theoretical calculations of the vibrational transition probabilities in hydrogen selenide 122 (1988) 375
Snijders, J.G., see P.M. Boerrigter 122 (1988) 357
Sotnikov, M.V., see Yu.A. Kuritsyn 122 (1988) 97
Stevens, B., Electron-donor–acceptor orbital correlations. VI. Selection rules for adiabatic intermolecular electron transfer 122 (1988) 347
Stolte, S., see C. Liedenbaum 122 (1988) 443
Subbi, J., Multidimensional Franck–Condon integrals in the case of strong normal coordinate mixing 122 (1988) 157

Tang, K.T., see Q.F. Pan 122 (1988) 193
Tarantelli, F., see J. Schirmer 122 (1988) 9
Toennies, J.P., see C. Nyeland 122 (1988) 337
Tomasi, J., see R. Cammi 122 (1988) 63

Ulitsky, N.I., B.M. Kharlamov and R.I. Personov, Effect of a strong magnetic field on S–S transitions of organic molecules in amorphous matrices via hole burning 122 (1988) 1

Varma, C.A.G.O., see P.C.M. Weisenborn 122 (1988) 147
Vojtík, J., see I. Paidarová 122 (1988) 89

Wallace, R. and J.P. Leroy, The determination of generalized Jacobi vectors (GJVs) for common types of small molecules 122 (1988) 75
Walmsley, S.H., see J.A. Gisby 122 (1988) 271
Warman, J.M., see P.C.M. Weisenborn 122 (1988) 147
Wayne, R.P., see J. Wildt 122 (1988) 463
Weisenborn, P.C.M., C.A.G.O. Varma, M.P. de Haas and J.M. Warman, Contributions from dipolar electronically excited molecules and mobile charge carriers to photoinduced transient dielectric loss of solutions of some aniline derivatives 122 (1988) 147
Werner, H.-J., see J. Senekowitsch 122 (1988) 375
Werner, H.-J., see U. Mänz 122 (1988) 387

Wildt, J., G. Bednarek, E.H. Fink and R.P. Wayne, Laser excitation of $O_2(b^1\Sigma_g^+, v'=0, 1, 2)$ – rates and channels of energy transfer and quenching 122 (1988) 463

Yamaguchi, Y., see M. Duran 122 (1988) 201

Zilch, A., see J. Senekowitsch 122 (1988) 375
Zioło, J., see J. Chrapeć 122 (1988) 471

LIST OF SUBJECTS

1 METHODS

1.1 Theoretical

1.1.1 Group theory and algebras *
1.1.2 Classical mechanics
1.1.3 Quantized field theory
1.1.4 Many body and quasiparticle approaches *
1.1.5 Coupling schemes and perturbative treatments *
1.1.6 Relativistic quantum mechanics *
1.1.7 Transport quantum mechanics
1.1.8 Equilibrium statistical mechanics *
1.1.9 Statistical mechanics of stationary states
1.1.10 Non-equilibrium thermodynamic and hydrodynamic theories
1.1.11 Ab initio schemes for stationary properties *
1.1.12 Computational and simulation methods *
1.1.13 Molecular dynamics and scattering theory *

1.2 Experimental

1.2.1 Magnetic resonances *
1.2.2 Cyclotron resonance
1.2.3 Microwave spectroscopy
1.2.4 Infrared spectroscopy *
1.2.5 Raman spectroscopy *
1.2.6 Visible and UV spectroscopy *
1.2.7 Fluorescence spectroscopy
1.2.8 Photoelectron and Auger spectroscopy *
1.2.9 X-ray spectroscopy
1.2.10 Electron impact spectroscopy *
1.2.11 Laser methods *
1.2.12 Picosecond spectroscopy *
1.2.13 Non-linear optical spectroscopy
1.2.14 Synchrotron spectroscopies
1.2.15 Coherent optical spectroscopy
1.2.16 Optical pumping
1.2.17 Multiple resonance spectroscopy *
1.2.18 Optoacoustic spectroscopy
1.2.19 Atomic and molecular beam techniques
1.2.20 Time-resolved experiments *
1.2.21 Mass spectrometry
1.2.22 Radiolysis
1.2.23 Mössbauer spectroscopy
1.2.24 X-ray, electron and neutron diffraction
1.2.25 Neutron scattering
1.2.26 Light scattering
1.2.27 Field emission and field ionization
1.2.28 Measurement of macroscopic variables *

2 OBJECTS

2.1 Bulk systems

2.1.1 Gases *
2.1.2 Supersonic beams *
2.1.3 Liquids neat
2.1.4 Liquid mixtures and solutions *
2.1.5 Crystals *
2.1.5.1 neat
2.1.5.2 mixed
2.1.6 Glasses
2.1.7 Liquid crystals
2.1.8 Polymers *
2.1.9 Semiconductors
2.1.10 Metals and alloys
2.1.11 Thin films
2.1.12 Surfaces *
2.1.13 Low-dimensional materials
2.1.14 Dielectrics *
2.1.15 Plasmas
2.1.16 Biological systems

2.2 Microscopic systems

2.2.1 Atoms *
2.2.2 Molecules (neutral and ionic) *
2.2.2.1 diatomic *
2.2.2.2 small polyatomics *
2.2.2.3 aromatics
2.2.2.4 other large *
2.2.2.5 polymeric and biological
2.2.3 Molecular aggregates *
2.2.3.1 dimers *
2.2.3.2 van der Waals molecules
2.2.3.3 clusters
2.2.3.4 complexes *
2.2.4 Free radicals (including hydronium and muonium) *
2.2.5 Quasiparticles (including excitons) *
2.2.6 Defects and impurities
2.2.7 Ions and charge carriers

* Denotes subjects covered in this volume

3 PHENOMENA

3.1 Molecular structure *
3.2 Vibrations and rotations of molecules *
3.3 Electronic structure and states *
3.4 Electric and magnetic properties *
3.5 Spin splittings *
3.6 Optical activity *
3.7 Molecular interactions *
3.8 Spectral bandshapes and intensities *
3.9 Coupling of electronic and nuclear motion
3.10 Energy transfer processes *
3.11 Molecular photophysical processes *
3.12 Intramolecular dynamics *
3.12.1 radiationless transitions
3.12.2 vibrational energy redistribution (including vibrational dissociation)
3.13 Luminescence spectra, yields and lifetimes
3.14 Coherence loss processes
3.15 Non-linear responses (including optical) *
3.16 Multiphoton phenomena
3.17 Reactions (including dissociation) *
3.17.1 gas phase *
3.17.2 condensed phase *
3.17.3 photochemical
3.18 Tunnelling
3.19 Electron transfer *
3.20 Positron annihilation
3.21 Ionization (including Rydberg states) *
3.22 Molecular motion (including diffusive)
3.23 Isotopic effects
3.24 Fluctuations and noise
3.25 Collective motion and excitations *
3.26 Surface effects and catalysis
3.27 Thermodynamic and transport properties
3.28 Structure of solids and liquids
3.29 Critical phenomena *
3.30 Phase transitions

SUBJECT INDEX TO VOLUME 122

METHODS

Theoretical

Group theory and algebras

Laser-induced molecular orientation effects in vibrational resonance-Raman spectroscopy, D.L. Andrews and N.P. Blake 122 (1988) 169
Electron-donor–acceptor orbital correlations. VI. Selection rules for adiabatic intermolecular electron transfer, B. Stevens 122 (1988) 347

Many body and quasiparticle approaches

Theoretical study of K-shell excitations in formaldehyde, J. Schirmer, A. Barth and F. Tarantelli 122 (1988) 9
Intermolecular energy transfer in infrared-laser-induced desorption, B. Fain, V. Fleurov and S.H. Lin 122 (1988) 17
A study of the valence orbitals of H_2S by electron momentum spectroscopy: quantitative comparisons using Hartree–Fock limit and correlated wavefunctions, C.L. French, C.E. Brion and E.R. Davidson 122 (1988) 247
A theoretical investigation of the variation with pressure of the ultraviolet absorption spectrum of crystalline anthracene, J.A. Gisby and S.H. Walmsley 122 (1988) 271
Diffusion-controlled kinetics of systems containing a finite number of reacting particles, V.L. Klochikhin and S.Ya. Pshezhetskii 122 (1988) 279
Calculation of rotational *g*-factors and magnetic susceptibilities of H_3^+, J. Oddershede and J.R. Sabin 122 (1988) 291

Coupling schemes and perturbative treatments

Contribution to the theory of time-resolved microwave-induced optical nuclear polarization. Theoretical extremum values for the induced polarization, J.P. Colpa 122 (1988) 29
Multidimensional Franck–Condon integrals in the case of strong normal coordinate mixing, J. Subbi 122 (1988) 157

Relativistic quantum mechanics

A relativistic LCAO Hartree–Fock–Slater investigation of the electronic structure of the actinocenes $M(COT)_2$, M=Th, Pa, U, Np and Pu, P.M. Boerrigter, E.J. Baerends and J.G. Snijders 122 (1988) 357

Equilibrium statistical mechanics

Laser-induced molecular orientation effects in vibrational resonance-Raman spectroscopy, D.L. Andrews and N.P. Blake 122 (1988) 169

Ab initio schemes for stationary properties

Relation between total energy and orbital energy sum in molecules: atomic and bonding contributions, G. Kemister and N.H. March 122 (1988) 39

Ab initio configuration interaction study of the Rydberg states of the hydroxymethyl radical CH_2OH, S. Rettrup, P. Pagsberg and C. Anastasi 122 (1988) 45

Decomposition of the interaction energy with counterpoise corrections to the basis set superposition error for dimers in solution. Method and application to the hydrogen fluoride dimer, R. Cammi, F.J. Olivares del Valle and J. Tomasi 122 (1988) 63

Analytic energy second derivatives for paired-excited multi-configuration self-consistent-field wavefunctions. Application of the PEM CSCF model to H_2O, CH_2, HCN, HCCH, H_2CO, NH_3, CH_4, and C_2H_4, M. Duran, Y. Yamaguchi, R.B. Remington and H.F. Schaefer III 122 (1988) 201

Jahn–Teller distortions of SiH_4^+ and $Si(CH_3)_4^+$, T. Kudo and S. Nagase 122 (1988) 233

A study of the valence orbitals of H_2S by electron momentum spectroscopy: quantitative comparisons using Hartree–Fock limit and correlated wavefunctions, C.L. French, C.E. Brion and E.R. Davidson 122 (1988) 247

Calculation of rotational *g*-factors and magnetic susceptibilities of H_3^+, J. Oddershede and J.R. Sabin 122 (1988) 291

How reliable is the theoretical structure of SiC_2?, A.J. Sadlej, G.H.F. Diercksen, J. Oddershede and J.R. Sabin 122 (1988) 297

Molecular structure and spectroscopic properties of carbodiimide (HN–C–NH), M.T. Nguyen, N.V. Riggs and L. Radom 122 (1988) 305

A relativistic LCAO Hartree–Fock–Slater investigation of the electronic structure of the actinocenes $M(COT)_2$, M=Th, Pa, U, Np and Pu, P.M. Boerrigter, E.J. Baerends and J.G. Snijders 122 (1988) 357

Theoretical calculations of the vibrational transition probabilities in hydrogen selenide, J. Senekowitsch, A. Zilch, S. Carter, H.-J. Werner, P. Rosmus and P. Botschwina 122 (1988) 375

The first excited triplet state of NH_3, U. Mänz, P. Rosmus, H.-J. Werner and P. Botschwina 122 (1988) 387

Theoretical investigation of the dissociation of OCS^{2+} in the process $OCS(X^1\Sigma^+)+h\nu \rightarrow OCS^{2+} \rightarrow CO^+(X^2\Sigma^+)+S^+(^4S)$, J. Ridard, B. Levy and P. Millié 122 (1988) 403

Structure, energetics, and vibrational spectra of H-bonded systems. Dimers and trimers of HF and HCl, Z. Latajka and S. Scheiner 122 (1988) 413

Computational and simulation methods

The interaction potential and diffusion coefficients of sodium in neon, Q.F. Pan, M.S. Bowers and K.T. Tang 122 (1988) 193

How reliable is the theoretical structure of SiC_2?, A.J. Sadlej, G.H.F. Diercksen, J. Oddershede and J.R. Sabin 122 (1988) 297

Modelling of repulsive potentials from charge density distributions: a new site–site model applied to inert gas atoms with the diatomic molecules H_2, N_2, O_2, C. Nyeland and J.P. Toennies 122 (1988) 337

Molecular dynamics and scattering theory

The determination of generalized Jacobi vectors (GJVs) for common types of small molecules, R. Wallace and J.P. Leroy 122 (1988) 75

Non-adiabatic interaction in the autoionizing singlet He^*–H_2 system, I. Paidarová and J. Vojtík 122 (1988) 89

The interaction potential and diffusion coefficients of sodium in neon, Q.F. Pan, M.S. Bowers and K.T. Tang 122 (1988) 193
Conformational analysis of 2-chloro-5,5-dimethyl-2-oxo-1,3,2-dioxaphosphorinane by molecular dynamics method. Vibrational dephasing and interaction-induced IR absorption, H. Abramczyk and J. Michalak 122 (1988) 317
Sub-picosecond time-resolved intramolecular electronic energy transfer in bichromophoric rhodamine dyes in solution, N.P. Ernsting, M. Kaschke, J. Kleinschmidt, K.H. Drexhage and V. Huth 122 (1988) 431

Experimental

Magnetic resonances

Contribution to the theory of time-resolved microwave-induced optical nuclear polarization. Theoretical extremum values for the induced polarization, J.P. Colpa 122 (1988) 29
Proton ENDOR spectra of phenanthrene–TCNB triplet traps in single crystals of naphthalene–TCNB, A.L. Maniero, C. Corvaja and L. Pasimeni 122 (1988) 327

Infrared spectroscopy

Tunable diode laser studies of collisionless infrared excitation of SF_6 and NH_3 molecules, Yu.A. Kuritsyn, G.N. Makarov, I. Pak and M.V. Sotnikov 122 (1988) 97
Conformational analysis of 2-chloro-5,5-dimethyl-2-oxo-1,3,2-dioxaphosphorinane by molecular dynamics method. Vibrational dephasing and interaction-induced IR absorption, H. Abramczyk and J. Michalak 122 (1988) 317
Multi-photon excitation of a beam of SF_6 molecules pumped and probed by cw CO_2 lasers, C. Liedenbaum, S. Stolte and J. Reuss 122 (1988) 443

Raman spectroscopy

Laser-induced molecular orientation effects in vibrational resonance-Raman spectroscopy, D.L. Andrews and N.P. Blake 122 (1988) 169
Conformational analysis of 2-chloro-5,5-dimethyl-2-oxo-1,3,2-dioxaphosphorinane by molecular dynamics method. Vibrational dephasing and interaction-induced IR absorption, H. Abramczyk and J. Michalak 122 (1988) 317

Visible and UV spectroscopy

Effect of a strong magnetic field on S–S transitions of organic molecules in amorphous matrices via hole burning, N.I. Ulitsky, B.M. Kharlamov and R.I. Personov 122 (1988) 1
Ab initio configuration interaction study of the Rydberg states of the hydroxymethyl radical CH_2OH, S. Rettrup, P. Pagsberg and C. Anastasi 122 (1988) 45
Optical absorption spectra, crystal field analysis, and electric dipole intensity parameters for europium in $Na_3[Eu(ODA)_3]\cdot 2NaClO_4\cdot 6H_2O$, M.T. Berry, C. Schwieters and F.S. Richardson 122 (1988) 105
Circular dichroism spectra and electronic rotatory strengths of the europium 4f→4f transitions in $Na_3[Eu(ODA)_3]\cdot 2NaClO_4\cdot 6H_2O$, M.T. Berry, C. Schwieters and F.S. Richardson 122 (1988) 125
Multidimensional Franck–Condon integrals in the case of strong normal coordinate mixing, J. Subbi 122 (1988) 157
Observation of excited state species due to N^+/N_2^+ and CH_3HgX (X=Cl, Br, I) collisions, V. Kushawaha, A. Michael and M. Mahmood 122 (1988) 183

Vibrationally autoionizing Rydberg states of NH_3, P.J. Miller, W.A. Chupka and J.H.D. Eland 122 (1988) 395
Dynamics of a polymer matrix probed by the ring closure of merocyanine, R. Richert 122 (1988) 455

Photoelectron and Auger spectroscopy
Vibrationally autoionizing Rydberg states of NH_3, P.J. Miller, W.A. Chupka and J.H.D. Eland 122 (1988) 395

Electron impact spectroscopy
A study of the valence orbitals of H_2S by electron momentum spectroscopy: quantitative comparisons using Hartree–Fock limit and correlated wavefunctions, C.L. French, C.E. Brion and E.R. Davidson 122 (1988) 247

Laser methods
Effect of a strong magnetic field on S–S transitions of organic molecules in amorphous matrices via hole burning, N.I. Ulitsky, B.M. Kharlamov and R.I. Personov 122 (1988) 1
Tunable diode laser studies of collisionless infrared excitation of SF_6 and NH_3 molecules, Yu.A. Kuritsyn, G.N. Makarov, I. Pak and M.V. Sotnikov 122 (1988) 97
Vibrational relaxation of $HBr(v=1)$ in D_2 between 300 and 140 K, D. Papadimitriou, H.V. Schwarz and B. Schramm 122 (1988) 141
Multi-photon excitation of a beam of SF_6 molecules pumped and probed by cw CO_2 lasers, C. Liedenbaum, S. Stolte and J. Reuss 122 (1988) 443
Laser excitation of $O_2(b\,^1\Sigma_g^+, v'=0, 1, 2)$ – rates and channels of energy transfer and quenching, J. Wildt, G. Bednarek, E.H. Fink and R.P. Wayne 122 (1988) 463

Picosecond spectroscopy
Sub-picosecond time-resolved intramolecular electronic energy transfer in bichromophoric rhodamine dyes in solution, N.P. Ernsting, M. Kaschke, J. Kleinschmidt, K.H. Drexhage and V. Huth 122 (1988) 431

Multiple resonance spectroscopy
Proton ENDOR spectra of phenanthrene–TCNB triplet traps in single crystals of naphthalene–TCNB, A.L. Maniero, C. Corvaja and L. Pasimeni 122 (1988) 327

Time-resolved experiments
Contribution to the theory of time-resolved microwave-induced optical nuclear polarization. Theoretical extremum values for the induced polarization, J.P. Colpa 122 (1988) 29
Contributions from dipolar electronically excited molecules and mobile charge carriers to photoinduced transient dielectric loss of solutions of some aniline derivatives, P.C.M. Weisenborn, C.A.G.O. Varma, M.P. de Haas and J.M. Warman 122 (1988) 147
Dynamics of a polymer matrix probed by the ring closure of merocyanine, R. Richert 122 (1988) 455
Laser excitation of $O_2(b\,^1\Sigma_g^+, v'=0, 1, 2)$ – rates and channels of energy transfer and quenching, J. Wildt, G. Bednarek, E.H. Fink and R.P. Wayne 122 (1988) 463

Measurement of macroscopic variables
Properties of the nonlinear dielectric effect in critical nitrobenzene in *n*-alkane solutions in a broad range of temperatures, J. Chrapeć, S.J. Rzoska and J. Zioło 122 (1988) 471

OBJECTS

Bulk systems

Gases

Vibrational relaxation of HBr(v=1) in D_2 between 300 and 140 K, D. Papadimitriou, H.V. Schwarz and B. Schramm 122 (1988) 141
The interaction potential and diffusion coefficients of sodium in neon, Q.F. Pan, M.S. Bowers and K.T. Tang 122 (1988) 193
Vibrationally autoionizing Rydberg states of NH_3, P.J. Miller, W.A. Chupka and J.H.D. Eland 122 (1988) 395

Supersonic beams

Tunable diode laser studies of collisionless infrared excitation of SF_6 and NH_3 molecules, Yu.A. Kuritsyn, G.N. Makarov, I. Pak and M.V. Sotnikov 122 (1988) 97
Vibrationally autoionizing Rydberg states of NH_3, P.J. Miller, W.A. Chupka and J.H.D. Eland 122 (1988) 395
Structure, energetics, and vibrational spectra of H-bonded systems. Dimers and trimers of HF and HCl, Z. Latajka and S. Scheiner 122 (1988) 413
Multi-photon excitation of a beam of SF_6 molecules pumped and probed by cw CO_2 lasers, C. Liedenbaum, S. Stolte and J. Reuss 122 (1988) 443

Liquid mixtures and solutions

Decomposition of the interaction energy with counterpoise corrections to the basis set superposition error for dimers in solution. Method and application to the hydrogen fluoride dimer, R. Cammi, F.J. Olivares del Valle and J. Tomasi 122 (1988) 63
Properties of the nonlinear dielectric effect in critical nitrobenzene in *n*-alkane solutions in a broad range of temperatures, J. Chrapeć, S.J. Rzoska and J. Zioło 122 (1988) 471

Crystals

Optical absorption spectra, crystal field analysis, and electric dipole intensity parameters for europium in $Na_3[Eu(ODA)_3]\cdot 2NaClO_4\cdot 6H_2O$, M.T. Berry, C. Schwieters and F.S. Richardson 122 (1988) 105
Circular dichroism spectra and electronic rotatory strengths of the europium 4f→4f transitions in $Na_3[Eu(ODA)_3]\cdot 2NaClO_4\cdot 6H_2O$, M.T. Berry, C. Schwieters and F.S. Richardson 122 (1988) 125
A theoretical investigation of the variation with pressure of the ultraviolet absorption spectrum of crystalline anthracene, J.A. Gisby and S.H. Walmsley 122 (1988) 271
Proton ENDOR spectra of phenanthrene–TCNB triplet traps in single crystals of naphthalene–TCNB, A.L. Maniero, C. Corvaja and L. Pasimeni 122 (1988) 327

Polymers

Dynamics of a polymer matrix probed by the ring closure of merocyanine, R. Richert 122 (1988) 455

Surfaces

Intermolecular energy transfer in infrared-laser-induced desorption, B. Fain, V. Fleurov and S.H. Lin 122 (1988) 17

Dielectrics
Contributions from dipolar electronically excited molecules and mobile charge carriers to photoinduced transient dielectric loss of solutions of some aniline derivatives, P.C.M. Weisenborn, C.A.G.O. Varma, M.P. de Haas and J.M. Warman 122 (1988) 147
Properties of the nonlinear dielectric effect in critical nitrobenzene in *n*-alkane solutions in a broad range of temperatures, J. Chrapeć, S.J. Rzoska and J. Zioło 122 (1988) 471

Microscopic systems

Atoms
Relation between total energy and orbital energy sum in molecules: atomic and bonding contributions, G. Kemister and N.H. March 122 (1988) 39
Observation of excited state species due to N^+/N_2^+ and CH_3HgX (X = Cl, Br, I) collisions, V. Kushawaha, A. Michael and M. Mahmood 122 (1988) 183
The interaction potential and diffusion coefficients of sodium in neon, Q.F. Pan, M.S. Bowers and K.T. Tang 122 (1988) 193
Modelling of repulsive potentials from charge density distributions: a new site–site model applied to inert gas atoms with the diatomic molecules H_2, N_2, O_2, C. Nyeland and J.P. Toennies 122 (1988) 337

Molecules (neutral and ionic)
Theoretical study of K-shell excitations in formaldehyde, J. Schirmer, A. Barth and F. Tarantelli 122 (1988) 9
Relation between total energy and orbital energy sum in molecules: atomic and bonding contributions, G. Kemister and N.H. March 122 (1988) 39
Contributions from dipolar electronically excited molecules and mobile charge carriers to photoinduced transient dielectric loss of solutions of some aniline derivatives, P.C.M. Weisenborn, C.A.G.O. Varma, M.P. de Haas and J.M. Warman 122 (1988) 147
Multidimensional Franck–Condon integrals in the case of strong normal coordinate mixing, J. Subbi 122 (1988) 157
Observation of excited state species due to N^+/N_2^+ and CH_3HgX (X = Cl, Br, I) collisions, V. Kushawaha, A. Michael and M. Mahmood 122 (1988) 183
Jahn–Teller distortions of SiH_4^+ and $Si(CH_3)_4^+$, T. Kudo and S. Nagase 122 (1988) 233

–diatomic
Vibrational relaxation of HBr(v=1) in D_2 between 300 and 140 K, D. Papadimitriou, H.V. Schwarz and B. Schramm 122 (1988) 141
Modelling of repulsive potentials from charge density distributions: a new site–site model applied to inert gas atoms with the diatomic molecules H_2, N_2, O_2, C. Nyeland and J.P. Toennies 122 (1988) 337
Laser excitation of $O_2(b\,^1\Sigma_g^+, v'=0, 1, 2)$ – rates and channels of energy transfer and quenching, J. Wildt, G. Bednarek, E.H. Fink and R.P. Wayne 122 (1988) 463

–small polyatomics
Theoretical study of K-shell excitations in formaldehyde, J. Schirmer, A. Barth and F. Tarantelli 122 (1988) 9
The determination of generalized Jacobi vectors (GJVs) for common types of small molecules, R. Wallace and J.P. Leroy 122 (1988) 75

Non-adiabatic interaction in the autoionizing singlet He^*-H_2 system, I. Paidarová and J. Vojtík 122 (1988) 89
Analytic energy second derivatives for paired-excited multi-configuration self-consistent-field wavefunctions. Application of the PEM CSCF model to H_2O, CH_2, HCN, HCCH, H_2CO, NH_3, CH_4, and C_2H_4, M. Duran, Y. Yamaguchi, R.B. Remington and H.F. Schaefer III 122 (1988) 201
A study of the valence orbitals of H_2S by electron momentum spectroscopy: quantitative comparisons using Hartree–Fock limit and correlated wavefunctions, C.L. French, C.E. Brion and E.R. Davidson 122 (1988) 247
Calculation of rotational *g*-factors and magnetic susceptibilities of H_3^+, J. Oddershede and J.R. Sabin 122 (1988) 291
How reliable is the theoretical structure of SiC_2?, A.J. Sadlej, G.H.F. Diercksen, J. Oddershede and J.R. Sabin 122 (1988) 297
Molecular structure and spectroscopic properties of carbodiimide (HN–C–NH), M.T. Nguyen, N.V. Riggs and L. Radom 122 (1988) 305
Theoretical calculations of the vibrational transition probabilities in hydrogen selenide, J. Senekowitsch, A. Zilch, S. Carter, H.-J. Werner, P. Rosmus and P. Botschwina 122 (1988) 375
The first excited triplet state of NH_3, U. Mänz, P. Rosmus, H.-J. Werner and P. Botschwina 122 (1988) 387
Vibrationally autoionizing Rydberg states of NH_3, P.J. Miller, W.A. Chupka and J.H.D. Eland 122 (1988) 395
Theoretical investigation of the dissociation of OCS^{2+} in the process $OCS(X\,^1\Sigma^+)+h\nu\rightarrow OCS^{2+}\rightarrow CO^+(X\,^2\Sigma^+)+S^+(^4S)$, J. Ridard, B. Levy and P. Millié 122 (1988) 403

–other large

Effect of a strong magnetic field on S–S transitions of organic molecules in amorphous matrices via hole burning, N.I. Ulitsky, B.M. Kharlamov and R.I. Personov 122 (1988) 1
An improved Sandorfy C method for permethylpolysilanes, A. Herman 122 (1988) 53
Tunable diode laser studies of collisionless infrared excitation of SF_6 and NH_3 molecules, Yu.A. Kuritsyn, G.N. Makarov, I. Pak and M.V. Sotnikov 122 (1988) 97

Molecular aggregates

–dimers

Decomposition of the interaction energy with counterpoise corrections to the basis set superposition error for dimers in solution. Method and application to the hydrogen fluoride dimer, R. Cammi, F.J. Olivares del Valle and J. Tomasi 122 (1988) 63
Structure, energetics, and vibrational spectra of H-bonded systems. Dimers and trimers of HF and HCl, Z. Latajka and S. Scheiner 122 (1988) 413

–complexes

Optical absorption spectra, crystal field analysis, and electric dipole intensity parameters for europium in $Na_3[Eu(ODA)_3]\cdot 2NaClO_4\cdot 6H_2O$, M.T. Berry, C. Schwieters and F.S. Richardson 122 (1988) 105
Proton ENDOR spectra of phenanthrene–TCNB triplet traps in single crystals of naphthalene–TCNB, A.L. Maniero, C. Corvaja and L. Pasimeni 122 (1988) 327
Electron-donor–acceptor orbital correlations. VI. Selection rules for adiabatic intermolecular electron transfer, B. Stevens 122 (1988) 347

A relativistic LCAO Hartree–Fock–Slater investigation of the electronic structure of the actinocenes $M(COT)_2$, M=Th, Pa, U, Np and Pu, P.M. Boerrigter, E.J. Baerends and J.G. Snijders 122 (1988) 357
Structure, energetics, and vibrational spectra of H-bonded systems. Dimers and trimers of HF and HCl, Z. Latajka and S. Scheiner 122 (1988) 413

Free radicals (including hydronium and muonium)
Ab initio configuration interaction study of the Rydberg states of the hydroxymethyl radical CH_2OH, S. Rettrup, P. Pagsberg and C. Anastasi 122 (1988) 45

Quasiparticles (including excitons)
A theoretical investigation of the variation with pressure of the ultraviolet absorption spectrum of crystalline anthracene, J.A. Gisby and S.H. Walmsley 122 (1988) 271

PHENOMENA

Molecular structure
An improved Sandorfy C method for permethylpolysilanes, A. Herman 122 (1988) 53
Analytic energy second derivatives for paired-excited multi-configuration self-consistent-field wavefunctions. Application of the PEM CSCF model to H_2O, CH_2, HCN, HCCH, H_2CO, NH_3, CH_4, and C_2H_4, M. Duran, Y. Yamaguchi, R.B. Remington and H.F. Schaefer III 122 (1988) 201
Jahn–Teller distortions of SiH_4^+ and $Si(CH_3)_4^+$, T. Kudo and S. Nagase 122 (1988) 233
How reliable is the theoretical structure of SiC_2?, A.J. Sadlej, G.H.F. Diercksen, J. Oddershede and J.R. Sabin 122 (1988) 297
Molecular structure and spectroscopic properties of carbodiimide (HN–C–NH), M.T. Nguyen, N.V. Riggs and L. Radom 122 (1988) 305
The first excited triplet state of NH_3, U. Mänz, P. Rosmus, H.-J. Werner and P. Botschwina 122 (1988) 387
Structure, energetics, and vibrational spectra of H-bonded systems. Dimers and trimers of HF and HCl, Z. Latajka and S. Scheiner 122 (1988) 413

Vibrations and rotations of molecules
The determination of generalized Jacobi vectors (GJVs) for common types of small molecules, R. Wallace and J.P. Leroy 122 (1988) 75
Molecular structure and spectroscopic properties of carbodiimide (HN–C–NH), M.T. Nguyen, N.V. Riggs and L. Radom 122 (1988) 305
Theoretical calculations of the vibrational transition probabilities in hydrogen selenide, J. Senekowitsch, A. Zilch, S. Carter, H.-J. Werner, P. Rosmus and P. Botschwina 122 (1988) 375
Structure, energetics, and vibrational spectra of H-bonded systems. Dimers and trimers of HF and HCl, Z. Latajka and S. Scheiner 122 (1988) 413

Electronic structure and states
Theoretical study of K-shell excitations in formaldehyde, J. Schirmer, A. Barth and F. Tarantelli 122 (1988) 9
Ab initio configuration interaction study of the Rydberg states of the hydroxymethyl radical CH_2OH, S. Rettrup, P. Pagsberg and C. Anastasi 122 (1988) 45
An improved Sandorfy C method for permethylpolysilanes, A. Herman 122 (1988) 53

Optical absorption spectra, crystal field analysis, and electric dipole intensity parameters for europium in $Na_3[Eu(ODA)_3]\cdot 2NaClO_4\cdot 6H_2O$, M.T. Berry, C. Schwieters and F.S. Richardson 122 (1988) 105
Circular dichroism spectra and electronic rotatory strengths of the europium 4f→4f transitions in $Na_3[Eu(ODA)_3]\cdot 2NaClO_4\cdot 6H_2O$, M.T. Berry, C. Schwieters and F.S. Richardson 122 (1988) 125
Analytic energy second derivatives for paired-excited multi-configuration self-consistent-field wavefunctions. Application of the PEM CSCF model to H_2O, CH_2, HCN, HCCH, H_2CO, NH_3, CH_4, and C_2H_4, M. Duran, Y. Yamaguchi, R.B. Remington and H.F. Schaefer III 122 (1988) 201
A study of the valence orbitals of H_2S by electron momentum spectroscopy: quantitative comparisons using Hartree–Fock limit and correlated wavefunctions, C.L. French, C.E. Brion and E.R. Davidson 122 (1988) 247
A relativistic LCAO Hartree–Fock–Slater investigation of the electronic structure of the actinocenes $M(COT)_2$, M=Th, Pa, U, Np and Pu, P.M. Boerrigter, E.J. Baerends and J.G. Snijders 122 (1988) 357
The first excited triplet state of NH_3, U. Mänz, P. Rosmus, H.-J. Werner and P. Botschwina 122 (1988) 387
Vibrationally autoionizing Rydberg states of NH_3, P.J. Miller, W.A. Chupka and J.H.D. Eland 122 (1988) 395
Theoretical investigation of the dissociation of OCS^{2+} in the process $OCS(X^1\Sigma^+)+h\nu\rightarrow OCS^{2+}\rightarrow CO^+(X^2\Sigma^+)+S^+(^4S)$, J. Ridard, B. Levy and P. Millié 122 (1988) 403

Electric and magnetic properties
Effect of a strong magnetic field on S–S transitions of organic molecules in amorphous matrices via hole burning, N.I. Ulitsky, B.M. Kharlamov and R.I. Personov 122 (1988) 1
Contributions from dipolar electronically excited molecules and mobile charge carriers to photoinduced transient dielectric loss of solutions of some aniline derivatives, P.C.M. Weisenborn, C.A.G.O. Varma, M.P. de Haas and J.M. Warman 122 (1988) 147
Calculation of rotational *g*-factors and magnetic susceptibilities of H_3^+, J. Oddershede and J.R. Sabin 122 (1988) 291
Proton ENDOR spectra of phenanthrene–TCNB triplet traps in single crystals of naphthalene–TCNB, A.L. Maniero, C. Corvaja and L. Pasimeni 122 (1988) 327
Properties of the nonlinear dielectric effect in critical nitrobenzene in *n*-alkane solutions in a broad range of temperatures, J. Chrapeć, S.J. Rzoska and J. Zioło 122 (1988) 471

Spin splittings
Contribution to the theory of time-resolved microwave-induced optical nuclear polarization. Theoretical extremum values for the induced polarization, J.P. Colpa 122 (1988) 29
Proton ENDOR spectra of phenanthrene–TCNB triplet traps in single crystals of naphthalene–TCNB, A.L. Maniero, C. Corvaja and L. Pasimeni 122 (1988) 327

Optical activity
Circular dichroism spectra and electronic rotatory strengths of the europium 4f→4f transitions in $Na_3[Eu(ODA)_3]\cdot 2NaClO_4\cdot 6H_2O$, M.T. Berry, C. Schwieters and F.S. Richardson 122 (1988) 125

Molecular interactions
Decomposition of the interaction energy with counterpoise corrections to the basis set superposition error for dimers in solution. Method and application to the hydrogen fluoride dimer, R. Cammi, F.J. Olivares del Valle and J. Tomasi 122 (1988) 63

Non-adiabatic interaction in the autoionizing singlet He^*-H_2 system, I. Paidarová and J. Vojtík 122 (1988) 89
The interaction potential and diffusion coefficients of sodium in neon, Q.F. Pan, M.S. Bowers and K.T. Tang 122 (1988) 193
Conformational analysis of 2-chloro-5,5-dimethyl-2-oxo-1,3,2-dioxaphosphorinane by molecular dynamics method. Vibrational dephasing and interaction-induced IR absorption, H. Abramczyk and J. Michalak 122 (1988) 317
Modelling of repulsive potentials from charge density distributions: a new site–site model applied to inert gas atoms with the diatomic molecules H_2, N_2, O_2, C. Nyeland and J.P. Toennies 122 (1988) 337

Spectral bandshapes and intensities
Optical absorption spectra, crystal field analysis, and electric dipole intensity parameters for europium in $Na_3[Eu(ODA)_3]\cdot 2NaClO_4\cdot 6H_2O$, M.T. Berry, C. Schwieters and F.S. Richardson 122 (1988) 105
Circular dichroism spectra and electronic rotatory strengths of the europium 4f→4f transitions in $Na_3[Eu(ODA)_3]\cdot 2NaClO_4\cdot 6H_2O$, M.T. Berry, C. Schwieters and F.S. Richardson 122 (1988) 125
Conformational analysis of 2-chloro-5,5-dimethyl-2-oxo-1,3,2-dioxaphosphorinane by molecular dynamics method. Vibrational dephasing and interaction-induced IR absorption, H. Abramczyk and J. Michalak 122 (1988) 317
Theoretical calculations of the vibrational transition probabilities in hydrogen selenide, J. Senekowitsch, A. Zilch, S. Carter, H.-J. Werner, P. Rosmus and P. Botschwina 122 (1988) 375

Energy transfer processes
Intermolecular energy transfer in infrared-laser-induced desorption, B. Fain, V. Fleurov and S.H. Lin 122 (1988) 17
Vibrational relaxation of $HBr(v=1)$ in D_2 between 300 and 140 K, D. Papadimitriou, H.V. Schwarz and B. Schramm 122 (1988) 141
Sub-picosecond time-resolved intramolecular electronic energy transfer in bichromophoric rhodamine dyes in solution, N.P. Ernsting, M. Kaschke, J. Kleinschmidt, K.H. Drexhage and V. Huth 122 (1988) 431
Laser excitation of $O_2(b\,^1\Sigma_g^+, v'=0, 1, 2)$ – rates and channels of energy transfer and quenching, J. Wildt, G. Bednarek, E.H. Fink and R.P. Wayne 122 (1988) 463

Molecular photophysical processes
Contribution to the theory of time-resolved microwave-induced optical nuclear polarization. Theoretical extremum values for the induced polarization, J.P. Colpa 122 (1988) 29
Laser-induced molecular orientation effects in vibrational resonance-Raman spectroscopy, D.L. Andrews and N.P. Blake 122 (1988) 169
Dynamics of a polymer matrix probed by the ring closure of merocyanine, R. Richert 122 (1988) 455

Intramolecular dynamics
The determination of generalized Jacobi vectors (GJVs) for common types of small molecules, R. Wallace and J.P. Leroy 122 (1988) 75
Multi-photon excitation of a beam of SF_6 molecules pumped and probed by cw CO_2 lasers, C. Liedenbaum, S. Stolte and J. Reuss 122 (1988) 443

Non-linear responses (including optical)
Laser-induced molecular orientation effects in vibrational resonance-Raman spectroscopy, D.L. Andrews and N.P. Blake 122 (1988) 169

Multiphoton phenomena
Tunable diode laser studies of collisionless infrared excitation of SF_6 and NH_3 molecules, Yu.A. Kuritsyn, G.N. Makarov, I. Pak and M.V. Sotnikov 122 (1988) 97
Multi-photon excitation of a beam of SF_6 molecules pumped and probed by cw CO_2 lasers, C. Liedenbaum, S. Stolte and J. Reuss 122 (1988) 443

Reactions (including dissociation)
Jahn–Teller distortions of SiH_4^+ and $Si(CH_3)_4^+$, T. Kudo and S. Nagase 122 (1988) 233
Theoretical investigation of the dissociation of OCS^{2+} in the process $OCS(X^1\Sigma^+)+h\nu \rightarrow OCS^{2+} \rightarrow CO^+(X^2\Sigma^+)+S^+(^4S)$, J. Ridard, B. Levy and P. Millié 122 (1988) 403

–gas phase
Observation of excited state species due to N^+/N_2^+ and CH_3HgX (X=Cl, Br, I) collisions, V. Kushawaha, A. Michael and M. Mahmood 122 (1988) 183
Laser excitation of $O_2(b^1\Sigma_g^+, v'=0, 1, 2)$ – rates and channels of energy transfer and quenching, J. Wildt, G. Bednarek, E.H. Fink and R.P. Wayne 122 (1988) 463

–condensed phase
Diffusion-controlled kinetics of systems containing a finite number of reacting particles, V.L. Klochikhin and S.Ya. Pshezhetskii 122 (1988) 279

Electron transfer
Electron-donor–acceptor orbital correlations. VI. Selection rules for adiabatic intermolecular electron transfer, B. Stevens 122 (1988) 347

Ionization (including Rydberg states)
Theoretical study of K-shell excitations in formaldehyde, J. Schirmer, A. Barth and F. Tarantelli 122 (1988) 9
Ab initio configuration interaction study of the Rydberg states of the hydroxymethyl radical CH_2OH, S. Rettrup, P. Pagsberg and C. Anastasi 122 (1988) 45
An improved Sandorfy C method for permethylpolysilanes, A. Herman 122 (1988) 53
Contributions from dipolar electronically excited molecules and mobile charge carriers to photoinduced transient dielectric loss of solutions of some aniline derivatives, P.C.M. Weisenborn, C.A.G.O. Varma, M.P. de Haas and J.M. Warman 122 (1988) 147
Observation of excited state species due to N^+/N_2^+ and CH_3HgX (X=Cl, Br, I) collisions, V. Kushawaha, A. Michael and M. Mahmood 122 (1988) 183
Jahn–Teller distortions of SiH_4^+ and $Si(CH_3)_4^+$, T. Kudo and S. Nagase 122 (1988) 233

Collective motion and excitations
An improved Sandorfy C method for permethylpolysilanes, A. Herman 122 (1988) 53

Critical phenomena
Properties of the nonlinear dielectric effect in critical nitrobenzene in *n*-alkane solutions in a broad range of temperatures, J. Chrapeć, S.J. Rzoska and J. Zioło 122 (1988) 471